TITLE: Specific Heat and Latent Heat in Finite and Infinite One-Component Plasmas

Specific Heat and Latent Heat in Finite and Infinite One-Component Plasmas

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Abstract. The phase transition from liquid to ordered state has been explored in Molecular Dynamics simulations of confined one-component plasma clouds (as in ion traps). The latent heat and specific heat have been extracted and compared with Coulombic matter. The transition temperature is found to be lower for finite systems than for infinite matter, and the difference depends on the number of confined particles.

A one-component plasma (OCP) is known to have a transition from a liquid to a solid phase at a temperature corresponding to $\Gamma \approx 170\text{-}180$ [1], where $\Gamma \equiv (q^2/a_{WS})/kT$, and a_{WS} is the Wigner-Seitz radius of the volume occupied by one ion. The behavior of the latent heat is discussed in the literature, (though the one plot of specific heat that has been published [2] omits the peak in the specific heat for the transition).

The configuration of finite, confined plasmas (fewer than 100,000 ions) shows a different type of ordering from that in infinite matter at low temperatures: concentric, equidistant shells with 2-dimensional ordering within the shells, instead of a bcc structure [3]. The question of how sharp these transitions are in the finite systems, and where they occur, has not previously been explored.

Molecular Dynamics simulations were carried out, first for a system of 10,000 ions confined in a static, isotropic harmonic well, with a confining force of F = -Kr. The system was cooled gradually to a temperature that corresponds to $\Gamma \approx 30{,}000$. The outer two shells for this system are shown in Fig. 1 together with the shell structure.

The potential energy of the system was extracted after equilibrium had been established. The potential energy is given by

$$U = 1/2K \sum_i r_i^2 + \sum_{i,j>i} q^2/r_{ij} \qquad (1)$$

where r_i is the radial distance from the origin and r_{ij} is the distance between two ions and q is the charge of the ions.

Then, temperature increases were applied by two different methods. In one, the temperature was simply increased by scaling up the velocities, and the system was allowed to equilibrate for some 40 plasma periods (with about 120 time steps in the

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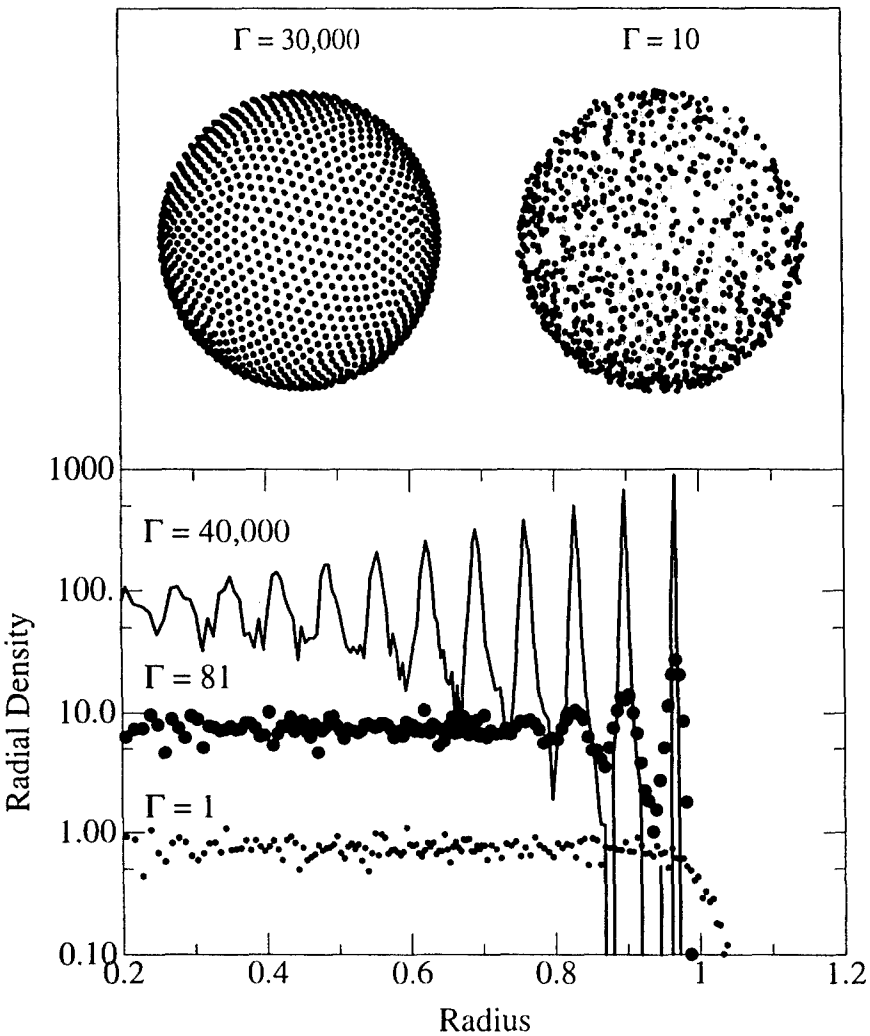

FIGURE 1. The upper part of the figure shows the outer layers of 10,000 ions. On the left is a very cold system with the outer shell shown in black, and the second shell in grey. On the right is a system in the liquid regime with no structure, with the selection of particles in the same radial regions. The lower part of the figure shows the radial density for three values of the temperature. The solid curve is a frozen, well-ordered system, the large points are in a region where the temperature is somewhat above the melting point and the small points are in the liquid regime.

simulation per plasma period). Then the following ~100 plasma periods were used to establish the new partition between kinetic energy (temperature) and potential energy. Alternatively, the temperature was increased in steps by assigning a random velocity to each particle picked from a Boltzmann distribution with the appropriate mean temperature, and then allowing the system to settle. This latter method seemed to allow the use of somewhat shorter time periods to establish a new equilibrium. The

two procedures gave very similar results. These times for equilibration and for establishing the averages were arrived at after some experimentation — a shorter time gave non-reproducible results. Attempts were also made at similar calculations in which the systems was cooled, rather than heated. Just as in laboratory experiments to determine the melting or freezing temperatures of materials, only the melting process seemed to give consistently reproducible results.

The results are shown in Fig. 2. At low temperatures, since the particles are oscillating about their equilibrium positions, the energy increments are distributed equally between kinetic and total energies. At a temperature, corresponding roughly to the above mentioned melting point in the infinite OCP, there is a step in potential energy, corresponding to the latent heat of melting. These data are displayed in a slightly different form in Fig. 3 where the upper part of the figure shows the potential energy divided by the kinetic energy for both the 10,000 ion simulation and the infinite OCP, the latter from [4]. The lower part of the figure shows the specific heat, taken as the increments in temperature divided by the corresponding increments in total energy. There appears to be a small difference in the transition energy, the point where the specific heat has its maximum value, in that the peak in the 10,000 ion system occurs at ~20% lower temperature: $\Gamma \approx 210$, instead of 173.

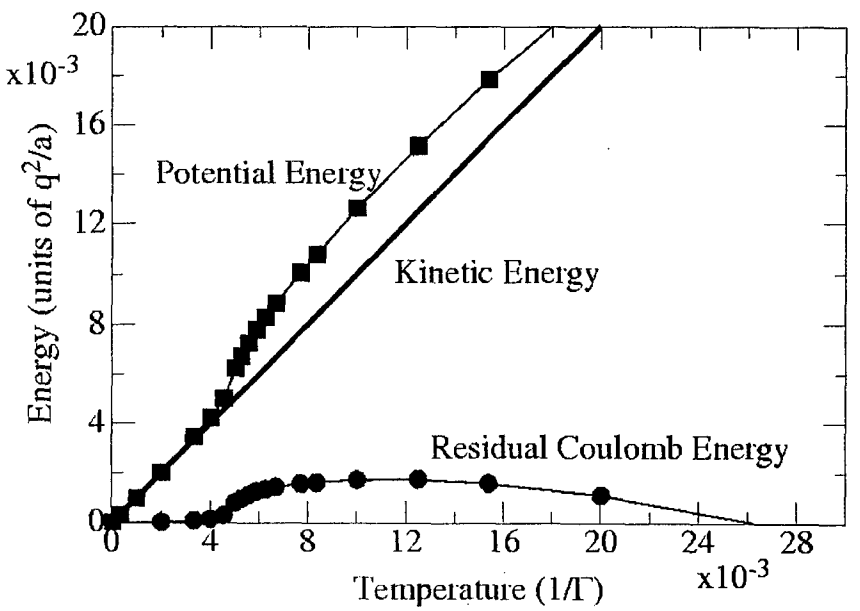

FIGURE 2. The potential energy in a 10,000 ion system is plotted as squares against the kinetic energy, in the same units of q^2/a_{WS}. At low temperature, the zero in potential energy is chosen arbitrarily as the value at $T = 0$. For $T < 0.005$ the particles oscillate about their equilibrium positions and the total energy is divided equally between the kinetic and potential energies. The deviation in the potential energy at $T \approx 0.005$ corresponds to the transition from an ordered to a disordered structure. At the bottom, the difference between the potential and kinetic energies is plotted.

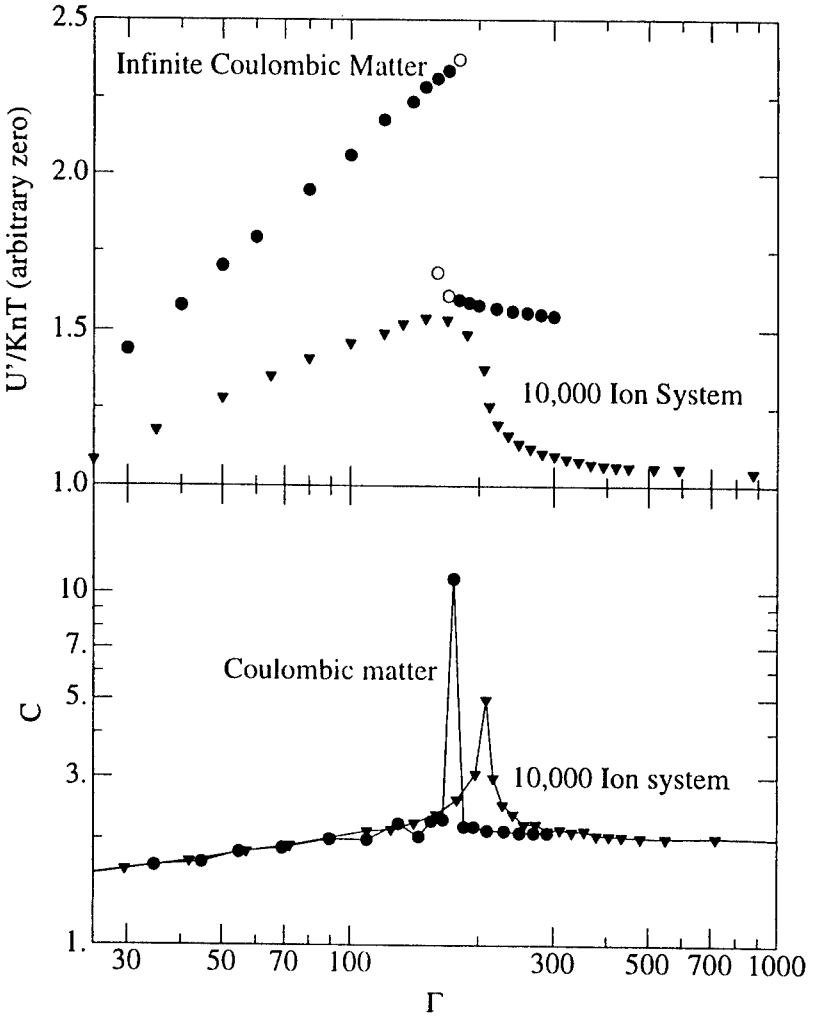

FIGURE 3. The upper part of the figure shows the total energy, U', divided by the temperature for infinite Coulombic matter [4] as circular dots, compared to the simulations for 10,000 ions as triangles. The origins on the vertical scale are displaced. On the right (low-temperature) part of the curve the ratio is constant for both, as expected. The lower part of the figure shows the specific heat C derived from the same sets of data.

Next, the different measures of ordering were investigated:

- the width of the shells,
- the related maxima in the radial densities for each shell,
- the heights of the maxima in the 2-dimensional correlation function g(r) within the shells,
- the heights of the maxima in the 3-dimensional g(r) over the entire volume of the cloud.

All of these showed the maximum rate of change near the transition temperature in the specific heat, and at a temperature lower than the transition temperature for the infinite OCP. This consistency is not surprising, since the ordering is the source of the latent heat. An example is shown in Fig. 4.

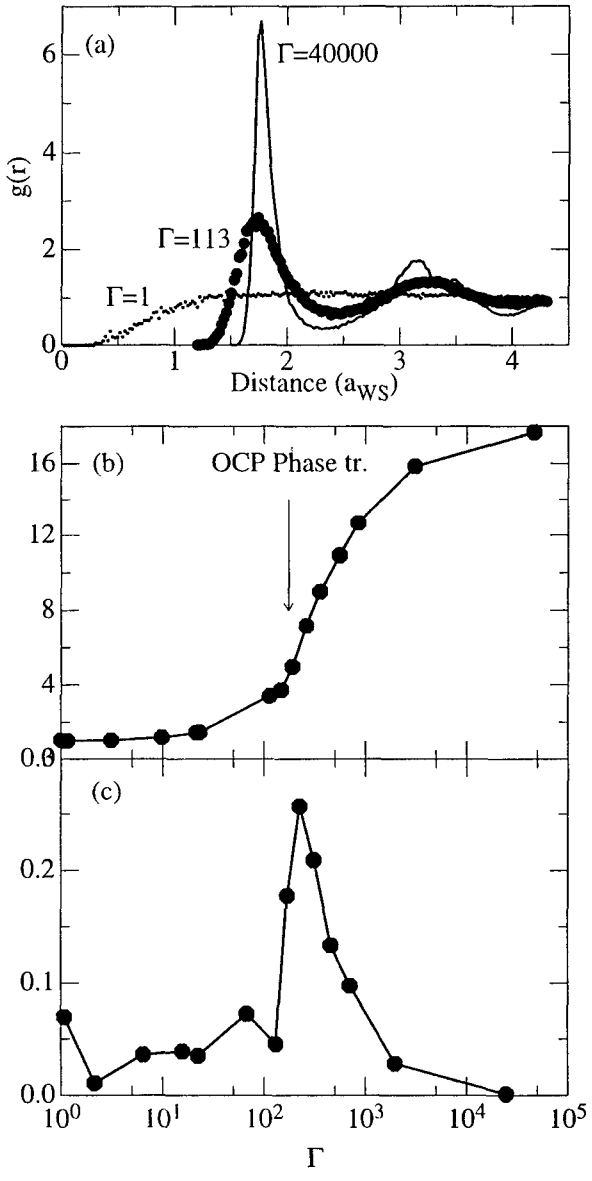

FIGURE 4. In (a) the 3-dimensional correlation function g(r) is plotted for three values of Γ, in (b) the ratio of the maximum in g(r) to the following minimum is shown, also as a function of Γ, while in (c) the derivative of this ratio is plotted.

In order to investigate the question of whether the lowering of the transition temperature is real or not, similar calculations were carried out for 1000 and 100 ions. These are displayed in Fig. 5. It is clear that the peaks in specific heat are broader and weaker in the smaller systems. For both 1000 and 100 ions the calculations were repeated several times in order to ascertain that the effects were reproducible. As is shown in the lower part of Fig. 5, there indeed appears to be a systematic trend in the transition temperature becoming lower for the smaller clusters.

Such a trend appears to have a simple explanation, in that ions on the surface do not see nearest neighbors on the outside, and thus their mobility is not constrained in the same way as for ions in the interior. Such effects are known to occur in atomic and molecular clusters (for instance for gold atoms [5]), but there the interactions are short range. One might expect, that with ionic clusters where the interaction is purely through the long-range Coulomb force, the effect might have a different character. The lower part of Fig. 5 shows that the transition temperature, as a function of the fraction of ions that are in the surface layer, seems to obey a simple dependence.

For real ion traps, the geometry considered here is close to that in Penning traps, where for the rotating cloud the effects of rotation at low temperature may be transformed away by the choice of the coordinate frame. The above simulations may therefore be expected to be directly tested there. The question of the transition temperatures in ions confined in rf-traps (Paul traps, and other configurations) is not necessarily so clear. The fact that the imposed rf motion does not cause appreciable heating of a cold plasma has been shown [6] but no further studies have been made. Therefore, a simulation was carried out for 1000 ions in rf confinement as described in [6]. In these systems a quasi-temperature is defined, that includes only motion that is aperiodic in the rf field: only motion that corresponds to displacements in complete rf periods are considered. The kinetic energy in the rf motion can be orders of magnitude higher. For calculations of specific heat, the potential energy of the system also needs to be known, and this clearly oscillates during the rf motion. Two methods were tried:

a) averaging the *potential energy* over complete rf cycles, or
b) averaging the *coordinates* of each ion and computing the potential energy corresponding to these average coordinates.

The two methods gave essentially identical results. One might have expected that because the method of confinement involves a continuous driven oscillation of all particles, plasmas confined in such a field might perhaps be more fragile and melt more easily (at lower temperatures) than those confined is static field. However, the specific heat from the simulations in the rf field peaked at a value of Γ that was consistent with the static calculations and no such effect was observed.

The values of specific heat much above the transition temperature could not be extracted from the rf-confined system because, as was shown in [6], at these temperatures there is increasing self-heating, "rf heating", from the coupling of the rf motion into the random heat of the plasma and to obtain meaningful results for these higher temperatures will require further study. However, it is clear that the rf motion does not appear to make systems confined in such an environment any more fragile with respect to melting than those confined in static fields.

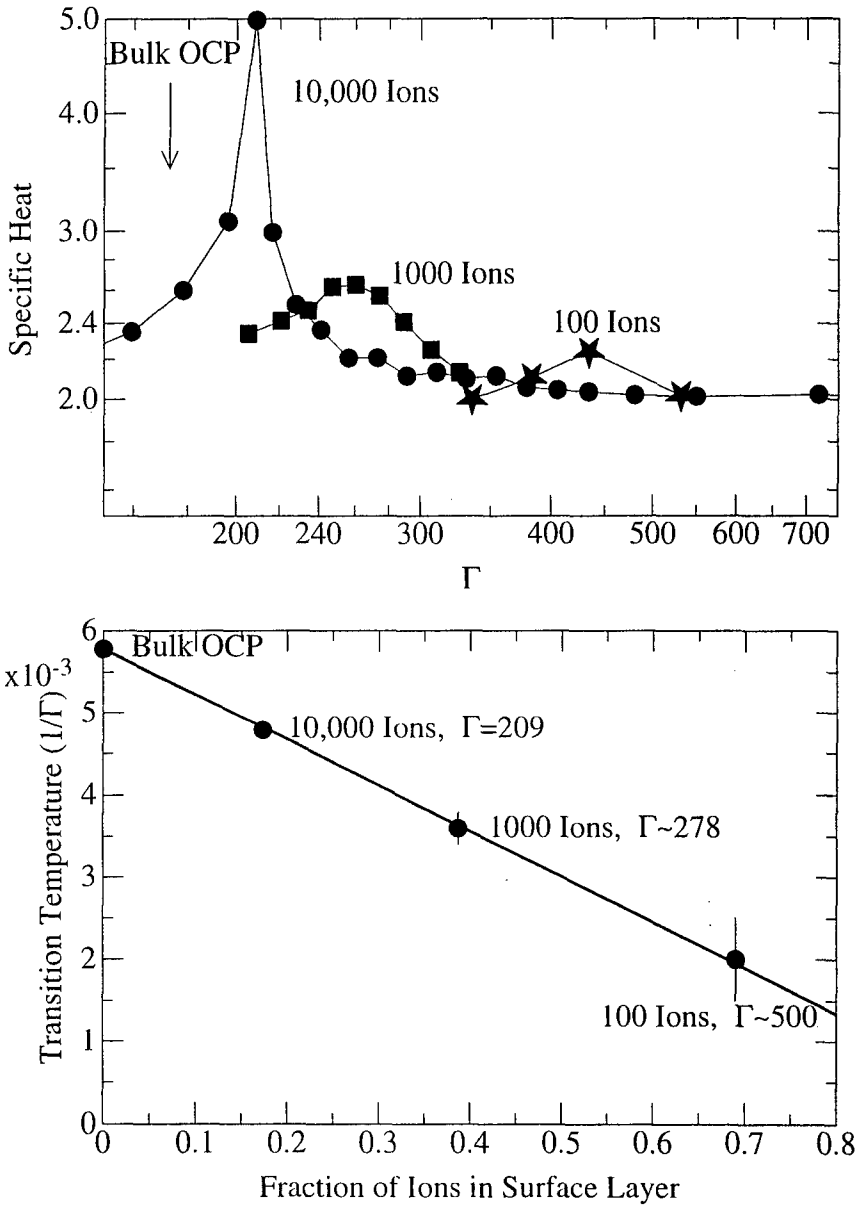

FIGURE 5. The upper part of the figure shows specific heats from simulations of 10,000, 1000 and 100 ions (circles, squares, and stars). The lower part of the figure shows the transitions temperatures (temperatures at which there is a peak in the specific heat) as a function of the number of ions in the surface layer for these systems. The line corresponds to $\Gamma = \Gamma_{OCP} \times (1 - 0.96 \times \text{fraction})$.

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